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Electron impact single and double ionization of He-like ions

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Abstract : We present in this communication the results of our calculation of TDCS and FDCS of (e,2e) and (e,3e) processes respectively on the He like ions at incident electron energy of 1099 eV. We have performed the calculation using distorted wave Born approximation (DWBA) formalism for (e,2e) process and three Coulomb (3C) wave approach for (e,3e) process in shake-off mechanism. We present the angular profiles of FDCS in coplanar asymmetric geometry as well as that of FDCS in constant θ_1 mode and discuss the role of atomic number Z on it. We also discuss the similarities and dissimilarities between (e,2e) and (e,3e) processes of He-like ions

Keywords : (e, 2e), (e, 3e), DWBA, 3 Coloumb wave approach, FDCS, TDCS

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1. Introduction

The ionization of atoms and ions by electron impact is one of the basic processes of atomic physics, with fundamental applications in different areas as astrophysics, plasma physics, fusion physics, surface science *etc*. The complex interactions involved in electron impact ionization of atoms and ions, is a challenging problem to understand. Fundamentally, an (e,2e) process is one where an electron, of well defined energy and momentum (E_i, K_i), is incident on a target, ionizes it and the outgoing electrons are detected in coincidence with their energies and angles resolved. A triple differential cross section (TDCS) is required to fully characterize the (e,2e) process for any given incident energy E_i. The TDCS $\sigma = d^3\sigma/(d\Omega_s\, d\Omega_1\, dE_1)$ is differential in two solid angles $d\Omega_s, d\Omega_1$ defined by the directions of the correlated electrons and is differential in the energy of one of the outgoing electrons. This ionization process is important for investigating the three-body problem, which consists of two outgoing electrons and the residual ion and is governed by the infinite long range Coulomb potential. However, more complex many-body problem, *i.e.* four-body problem, is encountered in experiments in which an incident electron on a target ejects two bound electrons and these two electrons as well as the scattered electron are detected coincidentally. Such type of coincident experiments are referred as a kinematically complete (e,3e) experiments in which informations about the collision dynamics, target electron momentum density and the correlated motion of the electrons can be obtained by measuring the five-fold differential cross section (FDCS), which is differential in solid angles of all the outgoing electrons and energies of the two ejected electrons.

The experimental and theoretical investigation of the (e,2e) processes on atoms have been done in different geometrical arrangements to get better understanding of the ionization mechanism as well as the characteristics of the targets. One can elucidate different features of the reaction mechanism by studying the (e,2e) process in different geometrical arrangements. One of them is coplanar asymmetric geometry (Ehrhardt geometry [1]). The coplanar asymmetric geometry is asymmetric in terms of energy or angle of the two outgoing electrons. In this geometrical arrangement TDCS is symmetric about the momentum transfer K, for any first order theory in non-relativistic regime, *i.e.* one gets a peak in the forward direction with a maximum at K, the direction in which an electron would move in a binary collision. There is also

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a smaller maximum in the direction of $-\boldsymbol{K}$, *i.e.* in the direction of the maximum recoil of the ion. Further, it has been shown by some workers [2–5] in the (e,3e) process that the centre of mass $\boldsymbol{K}_c = \boldsymbol{k}_1 + \boldsymbol{k}_2$ of the ejected electron (or the pair of the ejected electrons), where $\boldsymbol{k}_1$, $\boldsymbol{k}_2$ are the momenta of the ejected electrons, acts as an 'effective single particle' during the collision and as in (e,2e) process, binary and recoil peaks are observed in the FDCS *vs.* $\boldsymbol{K}_c$ direction curve in coplanar constant θ_{12} mode and this distribution is found to be symmetric about the direction of momentum transfer for any first order theory. Recently, Choubisa *et al* [4] have investigated this type of feature for He atom and shown the effect of post collision interaction (PCI) between the ejected electrons on the angular distribution of FDCS. Furthermore, the effect of second order projectile-target interaction on the symmetry of angular profile of FDCS has been investigated by Choubisa *et al.* [5].

In this communication, we present the results of our calculation of TDCS for (e,2e) process and FDCS for (e,3e) process in coplanar asymmetric and coplanar constant θ_{12} geometries respectively for He-like ions. Distorted Wave Born approximation (DWBA) formalism [6] is used for the calculation of TDCS while 3 Coulomb (3C) wave approach [7] is used for the calculation of FDCS. The present study helps us to understand the role of the nuclear charge Z on the angular profile of TDCS and FDCS, especially on the recoil peak. Further, it helps us to investigate the similarities and differences in the two processes.

2. Theory

2.1. *(e,2e) process :*

We have used distorted wave Born approximation (DWBA) formalism which is similar to the one developed by McCarthy and Weigold [6], to calculate triple differential cross section (TDCS) of the (e,2e) process on He-like ions. In this formalism following assumptions have been made :

(i) The incident and both the scattered and the ejected electrons are described by distorted waves.

(ii) The distorted wave for the incident electron is generated in the static exchange potential of the target and for the outgoing one in the static exchange potential of the residual ion.

(iii) Spin averaged static exchange potential and Hartree Fock wave function for target atom have been used.

We can express the triple differential cross section in distorted wave Born approximation as,

$$\frac{d^3\sigma}{d\Omega_s\, d\Omega_1\, dE_1} = (2\pi)^4 \frac{k_s k_1}{k_i} \sum_{av} \left(|f|^2 + |g|^2 - \mathrm{Re}(f^* g) \right)$$

where $\sum_{av}$ is the sum over the final and the average over the initial magnetic and spin degeneracy. k_i, k_s and k_1 are momenta of incident, scattered and ejected electron respectively and f and g are direct and exchange amplitudes respectively. The expressions for f and g are given as

$$f \equiv < X^{(-)}(k_s, r_t)\, X^{(-)}(k_1, r_1) | V | X^{(+)}(k_i, r_t) \psi_{nl} >,$$

$$g \equiv < X^{(-)}(k_s, r_1) X^{(-)}(k_1, r_t) | V | X^{(+)}(k_i, r_t) \psi_{nl} >,$$

and V represents the interaction potential between the incident and target electrons responsible for the ionization While ψ_{nl} is the atomic bound state orbital from which the electron is ionized. X^+ and X^- are the distorted wave for incident and outgoing electrons respectively The orbitals ψ_{nl} are taken from the wave functions of Clementi and Roetti [8]. The spin averaged static exchange potential is given as

$$V_E(r) = 0.5 \left(E + V_D(r) - \left\{ |E + V_D(r)|^2 - 2\pi \ell(r) \right\}^{\frac{1}{2}} \right),$$

where $\ell(r)$ is the electron density. The direct distorting potential $V_D(r)$ is obtained from the target radial orbital $\psi_{nl}(r)$ as

$$V_D(r) = \sum_{nl} N_{nl} \int dr' [u_{nl}(r')]^2 / r_>,$$

where $r_>$ is greater of r and r', N_{nl} is the number of electrons in each orbital n, l. The equivalent local ground state potential V_{00} is

$$V_{00} = V_D(r) + 0.5 \left(E + V_D(r) - \left\{ [E + V_D(r)]^2 - 2\pi \ell(r) \right\}^{\frac{1}{2}} \right).$$

2.2. *(e,3e) process :*

We present in this sub. section, the theoretical formalism to calculate the FDCS of (e,3e) process on He-like ions under the conditions of high electron impact energy and small excess ejected electrons energy. The present formalism has been developed with the following assumptions :

(i) The incident and scattered electrons are described by plane waves.

(ii) The bound electrons are described by the Le Sech wave functions [9].

(iii) The ejected electrons are described by the correlated approximate BBK [10] type wave function with effective charges as given by Lahmam-Bennani *et al* [11].

The five-fold differential cross section (FDCS) for the shake off mechanism in first Born approximation is given as,

$$\frac{d^5\sigma}{d\Omega_s\, d\Omega_1\, d\Omega_2\, dE_1\, dE_2} = (2\pi)^4 \frac{k_s k_1 k_2}{k_i} |T_{fi}|^2 \qquad (2)$$

where $d\Omega_s, d\Omega_1$ and $d\Omega_2$ are solid angle elements of scattered, first and second ejected electrons respectively while dE_1, dE_2 are the energy band pass of the ejected electrons and

$$T_{fi} = \frac{-1}{2\pi^2} \cdot \frac{1}{K^2} \cdot M_{fi} \,. \qquad (3)$$

We can express M_{fi} as

$$M_{fi} = \left\langle \psi_f(\boldsymbol{r}_1, \boldsymbol{r}_2) \left| -Z + \exp(i\boldsymbol{K}.\boldsymbol{r}_1) + \exp(i\boldsymbol{K}.\boldsymbol{r}_2) \right| \psi_i(\boldsymbol{r}_1, \boldsymbol{r}_2) \right\rangle, \qquad (4)$$

where $\boldsymbol{r}_1$ and $\boldsymbol{r}_2$ are the position vectors of the two ejected electrons with respect to the nucleus which is assumed to be located at the origin. We have used the target wave function $\psi_i(\boldsymbol{r}_1, \boldsymbol{r}_2)$, given by Le Sech wave function [9].

The ejected electrons are described by the correlated approximate BBK [10] type wave function $\psi_f(\boldsymbol{r}_1, \boldsymbol{r}_2)$ given by

$$\psi_f(\boldsymbol{r}_1, \boldsymbol{r}_2) = \frac{C}{\sqrt{2}} \left[\psi_{\boldsymbol{k}_1}(z_1, \boldsymbol{r}_1) \psi_{\boldsymbol{k}_2}(z_2, \boldsymbol{r}_2) + \psi_{\boldsymbol{k}_2}(z_2, \boldsymbol{r}_1) \psi_{\boldsymbol{k}_1}(z_1, \boldsymbol{r}_2) \right]$$

where

$$C = \exp(-\pi\eta/2)\, \Gamma(1 - i\eta)$$

and $\eta = \dfrac{1}{|\boldsymbol{k}_1 - \boldsymbol{k}_2|}$, which takes into account the correlation between the ejected electrons.

The Coulomb wave function $\psi_{\boldsymbol{k}_j}(z_j, \boldsymbol{r})$ of the outgoing electron is given by

$$\psi_{\boldsymbol{k}_j}(z_j, \boldsymbol{r}) = C_1 \exp(i\boldsymbol{k}_j \boldsymbol{r}_j)\; {}_1F_1\left(i\alpha_j, 1, -i(k_j r + \boldsymbol{k}_j \boldsymbol{r})\right)$$

where

$$C_1 = (2\pi)^{3/2}\, \Gamma(1 - i\alpha_j)\, \exp\left(\frac{-\pi\alpha_j}{2}\right)$$

and ${}_1F_1\left(i\alpha_j, 1, -i(k_j r + \boldsymbol{k}_j \boldsymbol{r})\right)$ is hypergeomentric function while $\Gamma(1 - i\alpha_1)$ is gamma function and $\alpha_j = -\dfrac{Z_j}{k_j}$.

The effective charges used [11] are given by the expressions :

$$Z_1 = Z + \frac{Z}{2}\frac{k_1}{k_s} - \frac{k_1}{|\boldsymbol{k}_s - \boldsymbol{k}_1|} \qquad (5a)$$

$$Z_2 = Z + \frac{Z}{2}\frac{k_2}{k_s} - \frac{k_2}{|\boldsymbol{k}_s - \boldsymbol{k}_2|} \qquad (5b)$$

The matrix element M_{fi} (4) can be expressed in terms of the integrals of the following two types :

$$I = \int e^{i\boldsymbol{K}.\boldsymbol{r}}\, e^{-ik_j.r - C_j}\; {}_1F_1(-i\alpha_j, 1, i(k_j r + \boldsymbol{k}_j.\boldsymbol{r}))\, d^3\boldsymbol{r} \qquad (6a)$$

and

$$I_2 = \int e^{ik_j r - C_j}\; {}_1F_1(-i\alpha_j, 1, i(k_j r + \boldsymbol{k}_j.\boldsymbol{r}))\, d^3\boldsymbol{r} \,. \qquad (6b)$$

We calculate the matrix element (4) numerically by using analytically evaluated integrals of the type (6a) and (6b) and for brevity explicit expressions are not given here.

3. Results and discussion

3.1. (e,2e) Process :

We have performed calculation of triple differential cross section (TDCS) for He-like ions (He, Li^+ and Be^{2+}) at incident electron energy 1099 eV in coplanar asymmetric geometry by keeping momentum transfer same for all the targets (K = 1 a.u.). We have plotted the angular profile of TDCS as a function of ejected electron angle (θ_1) for atom potential (dashed curve) as well as ion potential (solid curve) in Figure 1. The main features observed in the angular profile of TDCS are as follows :

(i) The binary and recoil peaks are observed in the direction of momentum transfer and opposite to it respectively for Li^+ and Be^{2+} targets using atomic potential in the calculation. However, the recoil peak for He atom (which is very shallow) is not observed in the direction opposite to the momentum transfer direction and found to be shifted towards lower angle (see dashed curves of Figure 1).

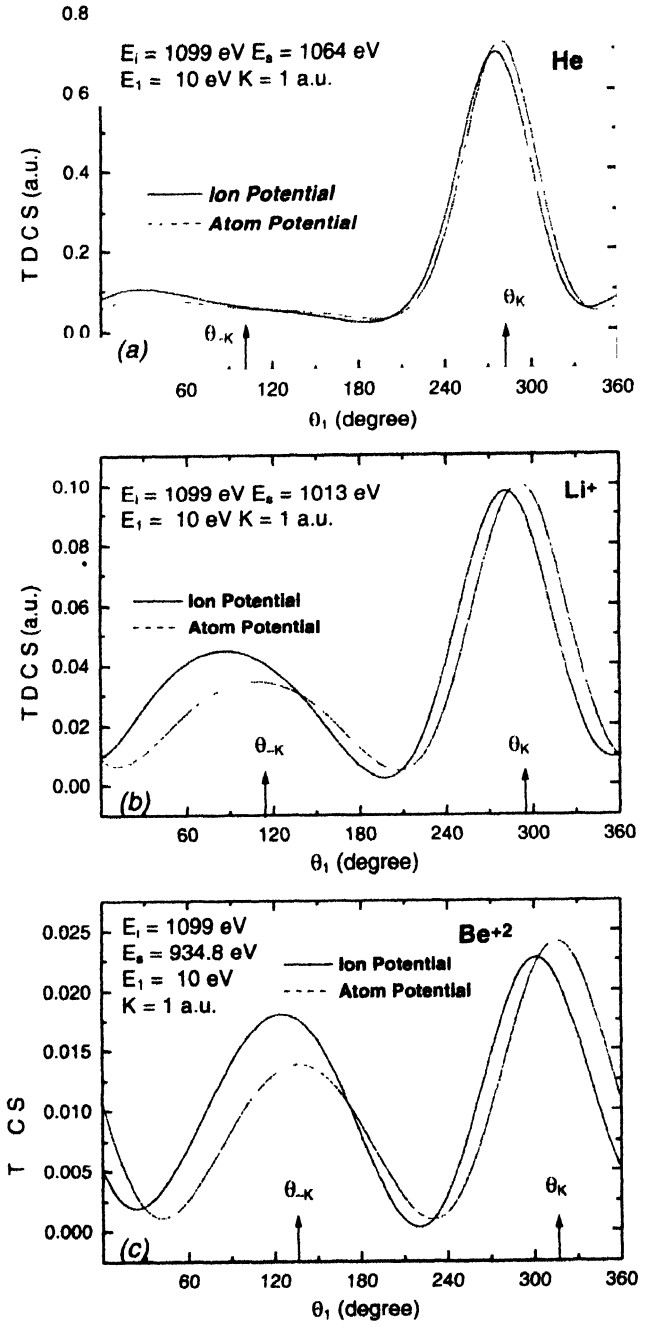

Figure 1. DWBA calculation of TDCS plotted as a function of ejected electron angle (θ_1) for He, Li^+ and Be^{2+} targets. Kinematics is displayed in each frame.

(ii) The angular profile of TDCS is found to be shifted on the inclusion of ion potential for all the three targets and thus the binary and recoil peaks are no more in the direction of momentum transfer and opposite to it respectively. Further, the shifting in the angular profile of TDCS is found to be more pronounced for higher Z targets (see solid curves of Figure 1).

(iii) We also observe that recoil peak gets enhanced and thus the ratio of TDCS of binary to recoil peak decreases with the increment of nuclear charge. This gives an indication of the importance of residual ion in the reaction mechanism of the (e,2e) process on He-like ions in which the electronic configuration is same and the only difference is in the strength of nuclear charge.

(iv) The binary peak is reduced and the recoil peak is enhanced on the inclusion of ion potential and thus the ratio of TDCS of binary to recoil peak decreases on its inclusion and further the decrement is more pronounced as nuclear charge is increased (see solid and dashed curves of Figure 1).

3.2. *(e,3e) process :*

We have performed calculation of five-fold differential cross section (FDCS) for He-like ions (H⁻, He and Li^+) at incident electron energy 1099 eV in coplanar constant θ_{12} geometrical mode by keeping momentum transfer same for all the targets (K = 1 a.u.) as we have chosen for (e,2e) process. In constant θ_{12} mode, the mutual angle between the ejected electrons is kept constant and FDCS is investigated with the variation of the angle of the bisector (θ) of the mutual angle. We have plotted the angular profile of FDCS as a function of θ for various θ_{12} angles in Figure 2 for above mentioned targets.

The main features observed in the angular profile of FDCS are as follows :

(i) As observed in the (e,2e) process the binary and recoil peaks are observed for all the θ_{12} angles for Li^+ target while for He target this feature is found to be observed for θ_{12} = 90° and 120° and this feature is nearly absent for lightest target (H^-). The origin of binary peak is due to the collision of the incident electron and the pair of the ejected electrons whereas the recoil peak is originated by the recoil of the pair of the ejected electrons by the massive ions [4].

(ii) For H^- target the recoil peak is nearly absent and the binary peak is split and hence two new peaks are formed near to the direction of momentum transfer. With the increment of nuclear charge as expected and observed in the (e,2e) process the recoil peak gets enhanced. Further, we observe that the feature of splitting of binary peak gets weakened for He target and it is absent for Li^+ target.

(iii) The angular profile of FDCS is found to be sensitive on the post collision interaction between the ejected electrons (*i.e.* on constant θ_{12} angles), particularly the recoil peak gets enhanced with the

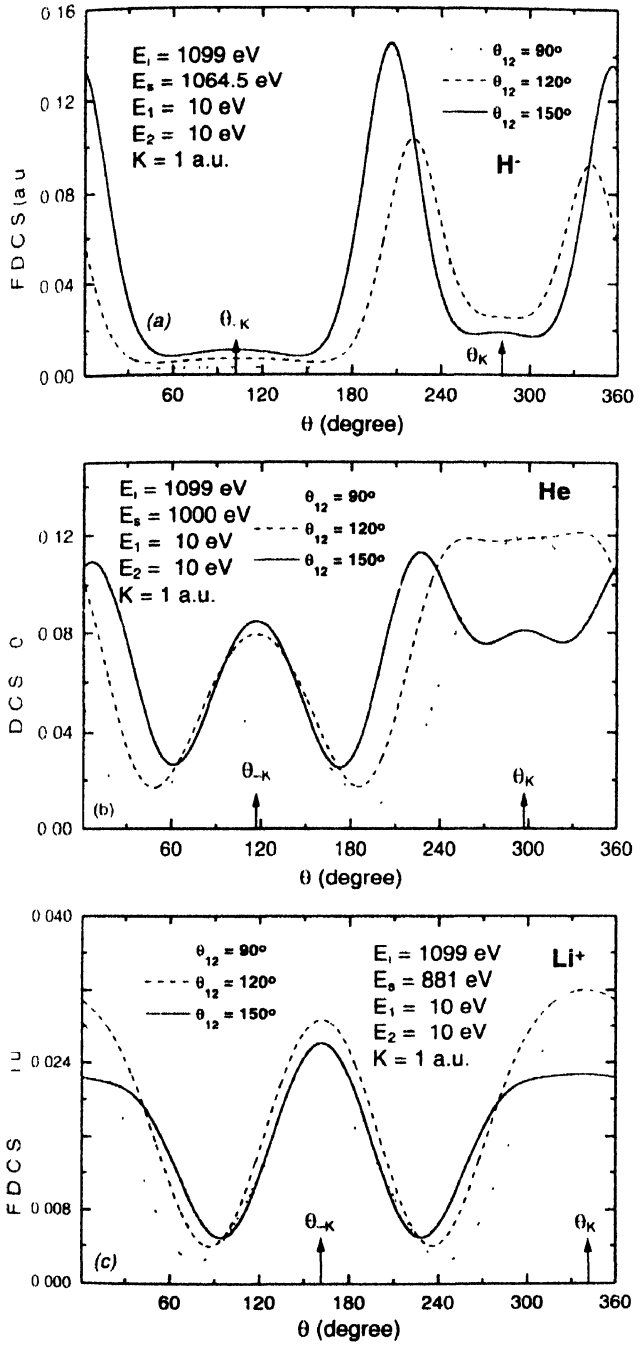

Figure 2. FDCS is plotted as a function of the angle of bisector (θ) of the constant mutual angle θ_{12} of the ejected electrons at various constant mutual angles as depicted in each frame of the Figure. The other kinematical parameters are shown in each frame.

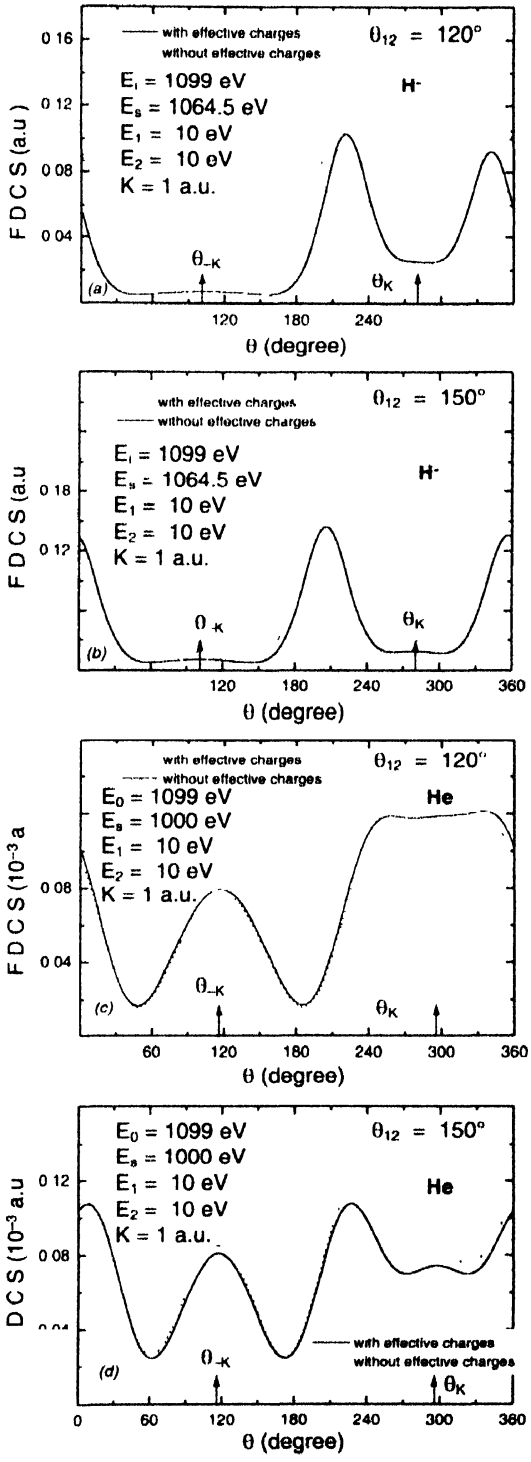

Figure 3. Same as in Figure 2 except for H and He atom. The full curve in each frame represents the FDCS calculated by incorporating effective charges while the dotted curve represents the FDCS calculated without using the effective charges.

increment of constant θ_{12} angles and consistent with our earlier study for He target only [4].

(iv) We also observe that the angular profile of FDCS is found to be symmetric about the direction of momentum transfer for all constant θ_{12} angles for Li^+ target while this symmetry is broken for other targets (see Figures 2(a)-(c)). The breaking of symmetry of FDCS about the direction of momentum transfer is due to non-first order effect, which comes in our calculation in the form of effective charges that includes the interaction between the scattered electron and the ejected electrons [11] (see eqs. 6(a) and 6(b)). We have plotted FDCS calculated using effective charges

(see solid curves of Figure 3) as well as that of using without effective charges (see dashed curves of Figure 3) as a function of θ for H^- and He targets. Our study clearly demonstrates that the breaking of the angular profile of FDCS is due to effective charges which includes non-first order interaction.

4. Conclusion

In conclusion, we have shown that the angular profile of the TDCS for (e,2e) process and that of FDCS for (e,3e) process of He-like ions is sensitive on the nuclear charge especially for the recoil peak which gets more pronounced for higher Z targets. Further it is observed that the binary peak in (e,3e) process gets split for He atom whereas for the (e,2e) process the splitting is not observed. We also observe that the ion potential shifts angular profile of the TDCS and this shifting is found to be more pronounced for higher Z targets. We have also investigated some kinematical conditions for H^- and He targets to see the effect of non-first order interaction on the angular profile of FDCS about the direction of momentum transfer.

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